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BLOW-UP OR NOT BLOW-UP AT THE HYPERBOLIC BOUNDARY FOR A CHEMISTRY SYSTEM ?

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ABSTRACT. We consider a system of conservation laws modeling heatless adsorption of a gaseous mixture with two species and instantaneous exchange kinetics. In this model the velocity is not constant because the sorption effect is taken into account. Exchanging the roles of the x , t variables we obtain a strictly hyperbolic system with a zero eigenvalue. We construct a solution with a velocity which blows up at the corresponding characteristic “hyperbolic boundary” $\{t = 0\}$. We introduce a fractional BV space to avoid this blow-up.

1. Introduction. This paper deals the blow up for an one dimensional 2×2 hyperbolic system of conservation laws related to a particular isothermal gas-solid chromatography process, called “Pressure Swing Adsorption” (PSA), with two species. Each of the two species simultaneously exists under two phases: a gaseous and movable one with a common velocity $u(t, x)$ and concentration $c_i(t, x) \geq 0$ and a solid (adsorbed) with concentration q_i , $i = 1, 2$. One may consult [3] for a precise description of the process and a survey on various related models. In gas chromatography, velocity variations accompany changes in gas composition: it is known as the sorption effect. Here, this effect is taken into account through a constraint: $c_1 + c_2 = 1$. We assume that mass exchanges between the mobile and the stationary phases are infinitely fast thus the two phases are constantly at composition equilibrium and the PSA system reads:

$$\partial_t(c_1 + q_1^*(c_1, c_2)) + \partial_x(u c_1) = 0, \quad (1)$$

$$\partial_t(c_2 + q_2^*(c_1, c_2)) + \partial_x(u c_2) = 0, \quad (2)$$

$$c_1 + c_2 = 1. \quad (3)$$

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Notice that c_1, c_2 must satisfy $0 \leq c_1, c_2 \leq 1$.

Adding (1) and (2) we get, thanks to (3):

$$\partial_t(q_1^*(c_1, c_2) + q_2^*(c_1, c_2)) + \partial_x u = 0.$$

Thanks to (3), we denote $c = c_1$ then $c_2 = 1 - c$ and the unknowns are the velocity u and the concentration c . We write the PSA system under the form:

$$\partial_x u + \partial_t h(c) = 0, \quad (4)$$

$$\partial_x(u c) + \partial_t I(c) = 0, \quad (5)$$

with

$$\begin{aligned} h(c) &= q_1^*(c, 1 - c) + q_2^*(c, 1 - c) = q_1(c) + q_2(c), \\ I(c) &= c + q_1^*(c, 1 - c) = c + q_1(c). \end{aligned}$$

Any equilibrium isotherm related to a given species is always non decreasing with respect to the corresponding concentration and non increasing with respect to the others thus $q_2' \leq 0 \leq q_1'$. We assume too that one gas is more active than the other: $h' < 0$. Then we have

$$0 \leq q_1' \leq -q_2' \quad (H1).$$

PSA system (4)-(5) is completed by initial and boundary data:

$$\begin{cases} c(0, x) = c_0(x) \in [0, 1], & x > 0, \\ c(t, 0) = c_b(t) \in [0, 1], & t > 0, \\ u(t, 0) = u_b(t) \geq \alpha, & t > 0, \text{ for some constant } \alpha > 0. \end{cases} \quad (6)$$

2. General properties for the PSA system. In this section, we recall briefly some properties of PSA system obtained in [1, 2, 4]. It is possible to analyse PSA system in terms of hyperbolic system provided we exchange the time and space variables. PSA system is strictly hyperbolic with variable x as the evolution variable: the two eigenvalues are 0 (linearly degenerate) and $\lambda = H(c)/u$ where

$$H(c) = 1 + q_1'(c) - ch'(c) = 1 + (1 - c)q_1'(c) - cq_2'(c) \geq 1. \quad (7)$$

The system is strictly hyperbolic with $u > 0$, but at ($t = 0, x = X_\infty$) it becomes degenerate hyperbolic because λ tends to 0 when u tends to $+\infty$. Then the boundary becomes twice characteristic. Using the function $f(c) = q_1(c) - ch(c)$, the right eigenvector associated to λ is genuinely nonlinear in each domain where $f'' \neq 0$. We also assume that

$$f'' > 0 \text{ everywhere} \quad (H2).$$

PSA system admits the two Riemann invariants c and $w = \ln(u) + g(c)$ where $g'(c) = -\frac{h'(c)}{H(c)} > 0$. Indeed, for smooth solutions we have: $\begin{cases} \partial_x c + \lambda \partial_t c = 0, \\ \partial_x w = 0. \end{cases}$

The Riemann invariant $W = uG(c) = e^w$ where $G(c) = \exp(g(c))$ plays a key-role in the blow up mechanism. If W is decreasing with respect to x we have $0 < uG(c) \leq u_b(t)G(c_b(t))$ thus

$$0 < u \leq \|u_b\|_\infty \sup_{c \in [0, 1]} G(c) / \inf_{c \in [0, 1]} G(c)$$

and u is bounded. Then if W is non decreasing with respect to x we can expect the velocity u to increase and blow up. Then an important assumption through out the paper is :

$$G'' < 0 \quad (H3).$$

It means that $-W$ is an admissible degenerate convex entropy for weak entropy solutions (with a zero entropy-flux). In contrary, notice that in some cases, for instance an inert gas and an active gas with a Langmuir isotherm as in [1], we have $G'' > 0$ then W is bounded and there is no blow up for the velocity in L^∞ .

There are two families of smooth entropies for the PSA system $u\psi(c)$ and $\phi(uG(c))$ where ϕ and ψ are any smooth real functions and the corresponding entropy fluxes satisfy $Q'(c) = h'(c)\psi(c) + H(c)\psi'(c)$. The first family is degenerate convex (in variables $(u, m = uc)$) provided $\psi'' \geq 0$. The second family is not always convex. Since $G'' < 0$, $-uG(c)$ is a degenerate convex entropy, with entropy flux $Q \equiv 0$. So, with $G'' < 0$ on $[0, 1]$, (c, u) has to satisfy, in the distribution sense $\frac{\partial}{\partial x}(uG(c)) > 0$.

3. The Riemann Problem. We solve the Riemann problem (1)-(2) with

$$\begin{cases} c(t, 0) = c^- \in [0, 1], & t < 0, \\ u(t, 0) = u^- > 0, \end{cases} \quad \begin{cases} c(t, 0) = c^+ \in [0, 1], & t > 0, \\ u(t, 0) = u^+ > 0, \end{cases} \quad (8)$$

We are classically looking for a selfsimilar solution: $c(t, x) = C(z)$, $u(t, x) = U(z)$, $z = \frac{t}{x}$. Since we assume that f is convex, there is no λ -contact discontinuity and the boundary Riemann problem is always solved by a simple wave (see [2]). A 0-wave appears on the line $\{t = 0\}$. As stated in [4], shock and rarefaction curves are monotonic.

Proposition 1. *Two distinct states U^- and U^0 are connected by a 0-contact discontinuity if and only if $c^- = c^0$. The solution of the Riemann problem for $x > 0$ is*

- $(c, u) = (c^-, u^-)$ for $t < 0$,
- a 0-contact discontinuity for $t = 0$,
- a λ wave for $t > 0$,

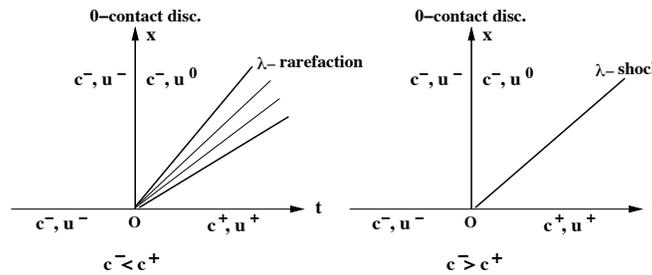


FIGURE 1. Solution of the Riemann problem when $f'' > 0$

As in a scalar conservation laws with piecewise constant data, no new shock can appear but shocks can disappear. It is a consequence of wave-interactions studied in [4]. We recall the following results concerning interactions:

- if a rarefaction interacts with a shock then we have a contact discontinuity and a rarefaction or a shock. If the shock and the rarefaction have the same strength (i.e. the same absolute variation of the concentration through the simple wave) we have only a contact discontinuity;

- if two shocks interact we obtain a contact discontinuity and a stronger shock;
- if a shock interacts with a contact discontinuity, we obtain a contact discontinuity and a shock with the same strength;
- if a rarefaction interacts with a contact discontinuity, we obtain a contact discontinuity and a rarefaction with the same strength.

More precisely, if a shock disappears after an interaction with a stronger rarefaction, by convention we follow the characteristic speed associated with the eigenvalue $\lambda = H(c)/u$, and the strength of the shock is 0.

We obtained in [1, 2] an existence result for weak global entropy solutions with large BV data for the concentrations and only L^∞ data for the velocity: as in [8], the zero eigenvalue makes the existence possible of stratified solutions in the sense that $u(t, x) = u_b(t) v(t, x)$ where v is as regular as the concentration c and more than the “initial” data u_b (see [4]). As we will see below, we cannot expect in general to have weak global entropy solutions with L^∞ data for the concentrations because it is possible, in that case, to build a blow up solution for some particular isotherms related for instance to ammonia or water vapor.

4. Temple class and PSA system. It is well known ([7]) that blow up cannot occur for Temple systems with L^∞ data. For PSA system we have:

Lemma 4.1. *PSA system (4)-(5) is a Temple system if and only if $\partial_x W = 0$ for the entropy solution of any Riemann problem.*

Proposition 2. *If $G'' = 0$ (for example if the two isotherms are linear or if $q_1 = 0$ with $q_2'' = 0$) then PSA system (4)-(5) is a Temple system.*

Remark 1. For an inert gas (for instance the first one: $q_1 = 0$) and an active gas with strictly convex isotherm ($q_2'' > 0$), PSA system is not in the Temple class. For example, it is the case if the active gas is the ammonia or the water vapor. For other examples, see [2, 4].

In the following, we use this supplementary assumption to avoid the Temple class:

PSA system (4)-(5) is not a Temple system (H4) .

5. The blow up solution. It is already known that systems of two hyperbolic conservation laws may blow up in the L^∞ norm. In [10], R. Young built a example involving two Burgers equations, linearly coupled at the two boundaries. In our example, we also loose the strict hyperbolicity of the system at the blow up point, but the blow up takes place only at the characteristic boundary $\{t = 0\}$ which becomes twice characteristic and only the velocity blows up. The context of our example is physically motivated and the various assumptions are physically relevant but a blow up along the x -axis at $t = 0$ is of course artificial. Nevertheless it illustrates what may occur when BV regularity is not ensured for the velocity at the physical boundary.

Theorem 5.1 (Blow up for velocity). *Assume (H1)-(H2)-(H3)-(H4). For any $T > 0$, $X_\infty > 0$, there exists a set of initial and boundary data (6) and a corresponding weak entropy solution on $[0, T] \times [0, X_\infty[$ of PSA system (4)-(5) such that $\|u\|_{L^\infty((0,T) \times (0, X_\infty))} = +\infty$.*

Actually the solution built to prove this theorem has special features.

- The velocity only blows up at the boundary $\{t = 0\}$ when $x \rightarrow X_\infty$, with arbitrary small data.
- $\forall X \in]0, X_\infty[$, $u, c \in L^\infty(0, T; BV(0, X)) \cap L^\infty(0, X; BV(0, T))$. The concentration c remains bounded while u blows up.
- Let Ω be a neighborhood of the critical point $(t = 0, x = X_\infty)$ such that $\Omega \subset [0, T] \times [0, X_\infty]$. Outside Ω , we can prove that (u, c) has a piecewise smooth structure, so the blow up occurs only at the boundary. Indeed, there is an accumulation of wave-interactions near $(t = 0, x = X_\infty)$.
- To build such solutions, we have necessarily to choose the boundary concentration $c_0(x) = c(0, x)$ not in $BV(0, X_\infty)$. Else there is no blow up, see [1, 2].
- The blow-up can be avoid with less constraint on initial data. Below, we introduce a fractional BV space to control the velocity at the boundary.

The main ingredient for the construction of the blow-up solution consists in the resolution of two consecutive boundary Riemann problems which leads to increase the velocity without increasing the concentrations.

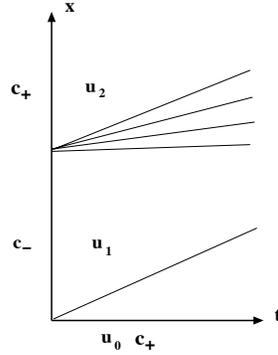


FIGURE 2. The two boundary Riemann problems

For the first boundary Riemann problem the data are (c_-, c_+, u_0) chosen in such a way that the solution is a shock wave and we set $u_1 = \mathcal{R}(c_-, c_+, u_0)$. For the second problem the data are (c_+, c_-, u_1) , the solution is necessarily a rarefaction wave and we set $u_2 = \mathcal{R}(c_+, c_-, u_1)$. With the assumptions, notice that for the shock curves we have $c_- < c_+$ (see [1]) and u is not monotonic along the process because $u_0 \leq u_2 \leq u_1$. We introduce now the *amplification coefficient* $\mathbf{R}(c_-, c_+)$ defined by $u_2 = \mathbf{R}u_0$.

Lemma 5.2. *We have the following properties:*

1. $\mathbf{R}(c_-, c_+) \geq 1$,
2. $\mathbf{R}(c_-, c_+) \equiv 1$ if and only if the system is in the Temple class,
3. \mathbf{R} is analytic then $\mathbf{R}(c_-, c_+) > 1$ almost everywhere in the domain $c_- < c_+$.

Notice that the commonly used isotherms are analytic, then \mathbf{R} also.

Let $N > 1$ be a fixed integer, $u_0 > 0$ and $0 = x_0 < x_1 < \dots < x_{2N-1} < X = x_{2N}$. We impose constant initial data and piecewise constant concentration at the boundary: for $0 < t < T$, $0 < x < X$, $k = 0, 1, \dots, N-1$:

$$\begin{cases} c(t, 0) = & \bar{c}, \\ u(t, 0) = & u_0, \\ c(0, x) = & \begin{cases} \underline{c}_k & \text{if } x_{2k} < x < x_{2k+1}, \\ \bar{c}_k & \text{if } x_{2k+1} < x < x_{2k+2}. \end{cases} \end{cases} \quad (9)$$

Riemann problems at the boundary are alternatively solved by a shock or a rarefaction and we construct the solution of PSA system with the Front Tracking Algorithm as in [4]:

Theorem 5.3. *With data (9) where \underline{c}_k and \bar{c}_k are constants such that*

$$0 < \underline{c} = \underline{c}_k < \bar{c} = \bar{c}_k < 1 \text{ with } \mathbf{R}(\underline{c}, \bar{c}) > 1$$

there exists an unique weak entropy solution in the class of piecewise Lipschitz functions. Furthermore, this solution has exactly N shock curves on $[0, T] \times [0, X]$.

There exists a domain Z (see Fig. 3), a neighborhood of the boundary $\{t = 0\}$ where boundary Riemann problems do not interact. In this domain Z we have an explicit solution. Let us denote by u_k the value of $u(x, 0^+)$ when $x_{k-1} < x < x_k$ for a given $k > 0$. Since $f'' > 0$ and $h' < 0$ we have N shocks emerging from $((x_{2k}, t = 0))_{k=0}^{N-1}$ and N rarefactions from $((x_{2k+1}, t = 0))_{k=0}^{N-1}$. Furthermore $u_{2k} < u_{2k+1}$, $u_{2k} < u_{2k+2} = \mathbf{R} u_{2k}$ and $u_{2k} = \mathbf{R}^k u_0$. Take $\delta > 0$ to discretize the rarefactions as in [4] and let shocks, rarefactions and contact discontinuities interact to obtain an approximate entropy solution on $[0, T] \times [0, X]$.

Notice that u is less regular than c because there are contact discontinuities emerging at each interaction between two waves.

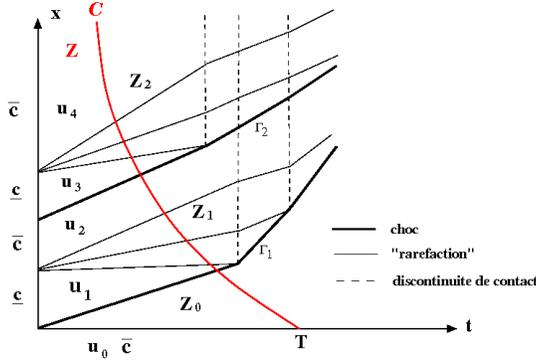


FIGURE 3. First interactions and free domain Z

We use data (9) with $N = +\infty$ i.e. $(x_k)_{k \in \mathbb{N}}$ is an increasing sequence such that $\lim_{k \rightarrow +\infty} x_k = X_\infty$. Then, the concentration remains bounded at the boundary but the BV norm of c and the L^∞ norm of u blow up at the boundary $t = 0$. Near $(t = 0, x = X_\infty)$, there is an accumulation of oscillations for the concentration and an accumulation of interactions between shocks and rarefactions.

The subset Z of $[0, T] \times [0, X_\infty[$ is a neighborhood of the vertical segment $\{0\} \times$

$[0, X_\infty[$. Indeed, the first interaction takes place at (t^1, x^1) : since a contact discontinuity propagates vertically, we have first to cut the set $\{t > t^1, x > x^1\}$. We do the same work, for all first interactions of the $2N$ Riemann problems issuing from the boundary. Then $Z = \{0 < x < X_\infty, 0 < t < z(x)\}$ where the function $z : [0, X_\infty] \rightarrow [0, T]$ is piecewise constant on $[0, X]$ for any $X < X_\infty$, non increasing, positive before X_∞ , $z(0) = T$, $z(X_\infty) = 0$. On Z , we exactly know the solution and

$$\lim_{(t,x) \in Z, x \rightarrow X_\infty} u(t, x) = +\infty.$$

Let $0 < X < X_\infty$. By previous construction, we get an unique piecewise smooth entropy solution U^X on $[0, T] \times [0, X]$. If $0 < X < Y < X_\infty$, we get U^Y and by uniqueness, $U^X = U^Y$ on $[0, T] \times [0, X]$. So, as for an ordinary differential equation, we can consider the unique maximal solution on $[0, T] \times [0, X_\infty[$. Before interaction between the solutions of the Riemann problems issuing from the boundary, we know explicitly U in Z . From geometric increasing of $u(0, x)$ when $x \rightarrow X_\infty$, we get a blow up for u at $t = 0, x = X_\infty$.

Furthermore, the characteristic slope $1/\lambda$ goes to infinity near $\{0\} \times \{X_\infty\}$ but outside a suitable “triangular neighborhood” of this point we get a determination domain where the solution has BV regularity and there is no blow up. This determination domain has the form

$$\mathcal{T} = \{(t, x); 0 < t < T, 0 < x < \min(X + \frac{t}{\lambda}, X_\infty)\}$$

for any X in $]0, X_\infty[$.

6. $BV^{1/3}$ space. We recall the classical result: shocks curves and rarefaction curves have a second order contact (see Theorem 8.2.2, page 209 in [9]). Then the amplification coefficient writes

$$R(c_-, c_+) = 1 + \mathcal{O}(|c_+ - c_-|^3). \quad (10)$$

According to the above cubic order, we introduce the fractional BV space: $BV^{1/3}$.

Definition 6.1 ($BV^{1/3}$). Let I be a non empty interval of \mathbf{R} . We note $S(I)$ the set of the subdivisions of I , that is the set of finite subsets $\sigma = \{x_0, x_1, \dots, x_n\} \subset I$ with $x_0 < x_1 < \dots < x_n$. Let u be a real function on I . The new total variation of u on I is defined by

$$TV^{1/3}u\{I\} = \sup_{\sigma \in S(I)} \sum_{i=1}^n |u(x_i) - u(x_{i-1})|^3.$$

The set $BV^{1/3}(I)$ is the set of functions $u : I \rightarrow \mathbf{R}$ such that $TV^{1/3}u\{I\} < +\infty$. We define the $BV^{1/3}$ semi-norm by $|u|_{BV^{1/3}(I)} = (TV^{1/3}u\{I\})^{1/3}$.

The following inclusions hold $BV(I) \subset BV^{1/3}(I) \subset L^\infty(I)$. More details and applications to conservation laws about spaces BV^s can be found in [6].

Theorem 6.2. *Under the same assumptions of Theorem 5.1, if c_0, c_b belong to $BV^{1/3}$ there is no blow up of the velocity at the characteristic boundary.*

Sketch of proof: we explain the proof for special set of initial and boundary value data. We use the same notations as in (9). The initial concentration c_0 in $BV^{1/3}$ yields $\sum_k |c_k - \bar{c}_k|^3 < +\infty$. To compute the speed at the hyperbolic characteristic boundary, we have the iterative relation: $u_{2(k+1)} = R(c_k, \bar{c}_k)u_{2k}$.

Thus, u is bounded at the boundary if and only if $\prod_k R(\underline{c}_k, \bar{c}_k)$ converges. With (10), we have the convergence.

Remark 2. If the initial concentration c_0 does not belong to $BV^{1/3}$, the blow-up can occur.

For instance, if the sequences \underline{c}_k and \bar{c}_k converge towards the same limit but $\sum_k |\underline{c}_k - \bar{c}_k|^3 = +\infty$ then $\prod_k R(\underline{c}_k, \bar{c}_k) = +\infty$ and the velocity blows up at the boundary.

The space $BV^{1/3}$ appears to be the critical space to control the blow-up at the boundary. So, we expect to have the following result:

Conjecture: if $u_b \in L^\infty$ and $c_0, c_b \in BV^{1/3}$ then there is existence of entropy solution for PSA system (4)-(5) in $BV^{1/3}$.

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